This thesis consists of six chapters. The first chapter gives an introduction to the field of low-dimensional magnetic and electronic systems and relevant numerical techniques. The recent developments in molecular magnets are highlighted. The numerical techniques are reviewed along with their advantages and disadvantages from the present perspective. Study of entanglement of a system can give a great insight into the system. At the last part of this chapter a general overview is given regarding entanglement, its measures and its significance in studying many-body systems.

Chapter 2 deals with the technique that has been developed by us for the full symmetry adaptation of non-relativistic Hamiltonians. It is advantageous both computationally and physically/chemically to exploit both spin and spatial symmetries of a system. It has been a long-standing problem to target a state which has definite total spin and also belongs to a definite irreducible representation of a point group, particularly for non-Abelian point groups. A very general technique is discussed in this chapter which is a hybrid method based on valence-bond basis and the basis of the z-component of the total spin. This technique is not only applicable to a system with arbitrary site spins and belonging to any point group symmetry, it is also quite easy to implement computationally. To demonstrate the power of the method, it is applied to the molecular magnetic system, Cu6Fe8, with cubic symmetry.

In chapter 3, the extension of the previous hybrid technique to electronic systems is discussed. The power of the method is illustrated by applying it to a model icosahedral half-filled electronic system. This model spans a huge Hilbert space (dimension 1,778,966) and is in the largest non-Abelian point group. All the eigenstates of the model are obtained using our technique.

Chapter 4 deals with the thermodynamic properties of an important class of single-chain magnets (SCMs). This class of SCMs has alternate isotropic spin-1/2 units and anisotropic high spin units with the anisotropy axes being non-collinear. Here anisotropy is assumed to be large and negative, as a result, anisotropic units behave like canted spins at low temperatures; but even then simple Ising-type model does not capture the essential physics of the system due to quantum mechanical nature of the isotropic units. A transfer matrix (TM) method is developed to study statistical behavior of this class of SCMs. For the first time, it is also discussed in detail that how weak inter-chain interactions can be treated by a TM method. The finite size effect is also discussed which becomes important for low temperature dynamics. This technique is applied to a real helical chain magnet, which has been studied experimentally.

In the fifth chapter a bipartite entanglement entropy of finite systems is studied using exact diagonalization techniques to examine how the entanglement changes in the presence of long-range interactions. The ParieserParrPople model with long-range interactions is used for this purpose and corresponding results are compared with those for the Hubbard and Heisenberg models with short-range interactions. This study helps understand why the density matrix renormalization group (DMRG) technique is so successful even in the presence of long-range interactions in the PPP model. It is also investigated if the symmetry properties of a state vector have any significance in relation to its entanglement. Finally, an interesting observation is made on the entanglement profiles of different states, across the full energy spectrum, in comparison with the corresponding profile of the density of states.

The entanglement can be localized between two noncomplementary parts of a many-body system by performing local measurements on the rest of the system. This localized entanglement (LE) depends on the chosen basis set of measurement (BSM). In this chapter six, an optimality condition for the LE is derived, which would be helpful in finding optimal values of the LE, besides, can also be of use in studying mixed states of a general bipartite system. A canonical way of localizing entanglement is further discussed, where the BSM is not chosen arbitrarily, rather, is fully determined by the properties of a system. The LE obtained in this way, called the localized entanglement by canonical measurement (LECM), is not only easy to calculate practically, it provides a nice way to define the entanglement length. For spin-1/2 systems, the LECM is shown to be optimal in some important cases. At the end of this chapter, some numerical results are presented for $j_1 - j_2$ spin model to demonstrate how the LECM behaves.